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On the definition of temperature in dense granular media

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In this Letter we report the measurement of a pseudo-temperature for compacting granular media on the basis of the Fluctuation-Dissipation relations in the aging dynamics of a model system. From the violation of the Fluctuation-Dissipation Theorem an effective temperature emerges (a dynamical temperature T_{dyn}) whose ratio with the equilibrium temperature T_d^{eq} depends on the particle density. We compare the results for the Fluctuation-Dissipation Ratio (FDR) T_{dyn}/T_d^{eq} at several densities with the outcomes of Edwards' approach at the corresponding densities. It turns out that the FDR and the so-called Edwards' ratio coincide at several densities (very different ages of the system), opening in this way the door to experimental checks as well as theoretical constructions.(PACS: 05.70.Ln, 05.20.-y, 45.70.Cc)

The study of compact granular matter through statistical physics tools is the subject of a sustained interest [1]. Granular media enter only partially in the framework of equilibrium statistical mechanics and their dynamics constitutes a very complex problem of non-equilibrium, which poses novel questions and challenges to theorists and experimentalists. The very possibility to construct a coherent statistical mechanics for these systems is still matter of debate, although everybody agrees that such an approach, if possible, would allow for a much deeper and global understanding of the problem.

One of the main obstacles in this direction is the non-thermal character of these systems: thermal energy is so negligibly small with respect to other energy contributions (e.g. potential energy) that for all the practical purposes these systems live virtually at zero temperature. One of the most important consequences is that, unless perturbed in some way (e.g. driving energy into the system), a granular system cannot explore spontaneously its phase space but it remains trapped in one of the numerous metastable configurations. Understanding the structure of the phase space which is left invariant by the dynamics is then crucial for the construction of a thermodynamical description of these non-thermal systems.

A very ambitious approach, in this direction, has been put forward by S. Edwards and co-workers [2, 3], by proposing an equivalent of the microcanonical ensemble: macroscopic quantities in a jammed situation should be obtained by a flat average over all *blocked configurations* (i.e. in which every grain is unable to move) of given volume, energy, etc... The strong assumption here is that all blocked configurations are treated as equivalent and have the same weight in the measure. This approach, based on the idea of describing granular material with *a small number of parameters*, leads to the introduction of an entropy S_{edw}, given by the logarithm of the number of blocked configurations of given volume, energy, etc., and its corresponding density $s_{edw} \equiv S_{edw}/N$. Associated with this entropy are the state variables such as 'compactivity' $\mathcal{X}^{-1} = \frac{\partial}{\partial V} S_{edw}(V)$ and 'temperature' $T^{-1} = \frac{\partial}{\partial E} S_{edw}(E)$.

Very recently, important progresses in this direction have been reported in various contexts: a tool to systematically construct Edwards' measure, defined as the set of blocked configurations of a given model, was proposed in [4, 5]; it was used to show that the outcome of the aging dynamics of the Kob-Andersen model (a kinetically constrained lattice gas model) was correctly predicted by Edwards' measure. Moreover, the validity and relevance of Edwards' measure have been demonstrated for one-dimensional phenomenological models [6], for spin models with "tapping" dynamics [7], and for sheared hard spheres [8].

In this Letter we focus on the definition of a pseudo-temperature for granular media on the basis of the Fluctuation-Dissipation relations in the out-of-equilibrium, aging, dynamics of a model system [9], and on its relation to Edwards' measure. From the violation of the Fluctuation-Dissipation Theorem an effective temperature emerges (from now onward indicated as dynamical temperature T_{dyn}) whose ratio with the equilibrium temperature T_d^{eq} depends on the particle density. We compare the results for the Fluctuation-Dissipation Ratio (FDR) T_{dyn}/T_d^{eq} at several densities with the outcomes of Edwards' approach at the corresponding densities. It turns out that the FDR and the so-called Edwards' ratio coincide at several densities (very different ages of the system), opening in this way the door to experimental checks as well as theoretical constructions.

It is interesting to mention recent approaches that are complementary to ours. On the one hand, in the context of aging supercooled liquids, the inherent structure strategy does not address the question of a determination of a static distribution, but promising results show that this measure, if it exists, is insensitive to the details of the

thermal history [10]. The link between this strategy and Edwards' measure has been discussed in [5, 11]. On the other hand, recent works on the possibility of a dynamical definition of temperature have focused on sheared, stationary systems [12, 13]. These studies are clearly complementary to the present one, which addresses the problem of the relation between the value of T_{dyn} and a static measure, in aging (non-stationary) systems.

The model we consider is a version of the "Tetris" model [9], which has been shown to reproduce several features of granular media like aging [14, 15], memory [16], self-structuring [17] etc. In the framework of this model, some of us have already provided one of the first evidences of the validity of Edwards' measure [5].

We focus in particular on an homogeneous system with no preferential direction in order to avoid any kind of instability or large-scale structure formation [17]. The case with gravity which imposes a preferential direction will be discussed elsewhere [18]. In the version of the model we use, "T"-shaped particles diffuse on a square lattice, with the only constraint that no superposition is allowed: for two nearest-neighbor particles, the sum of the arms oriented along the bond connecting the two particles has to be smaller than the bond length (for each particle, the three arms of the 'T" have length $\frac{3}{4}d$, where d sets the bond size on the square lattice). The maximum density allowed is then $\rho_{max} = 2/3$. This model represents a clear example of a non-thermal system. The Hamiltonian is zero and the temperature itself is therefore irrelevant at equilibrium, only its ratio with an imposed chemical potential being important.

The out-of-equilibrium compaction dynamics without gravity is implemented as follows: starting from an empty lattice, particles are randomly deposited, without diffusion and without violation of the geometrical constraints. This random sequential absorption process yields a reproducible initial density of $\rho \approx 0.547$. Alternating diffusions and additions of particles are then attempted, allowing to increase the density of the system, which remains homogeneous in the process. In order to overcome the problem related to the simulation of slow processes and obtain a reasonable number of different realizations to produce clean data, we have devised a fast algorithm (in the spirit of Bortz-Kalos-Lebowitz algorithm [19]) where the essential ingredient is the updating of a list of mobile particles (whose number is n_{mob}). At each time step one selects a mobile particle and move it in the direction chosen only if no violation of the constraints occurs. The time is incremented of an amount $\Delta t = 1/n_{mob}$. We refer to [18] for the details of the fast algorithm.

We have simulated lattices of linear size $L = 50,\ 100,\ 200$, in order to ensure that finite-size effects were irrelevant. We have chosen periodic boundary conditions on the lattice, having verified that other types of boundary conditions (e.g closed ones) gave the same results.

During the compaction, we monitor the following quantities: the density of particles $\rho(t)$, the density of mobile particles $\rho_{mob}(t)$. Moreover in order to establish the Fluctuation-Dissipation relations we measure the mean square displacement $B(t+t_w, t_w)$ and the integrated response function $\chi(t+t_w, t_w)$. The mean square displacement is defined as

$$B(t+t_w, t_w) \;=\; \frac{1}{N}\sum_{i=0}^{N}\sum_{r=x,y}\langle\,[r_i(t+t_w, t_w) - r_i(t_w)]^2\rangle$$

where N is the number particles present in the system at time t_w, r_i is the coordinate (x or y) of the i-th particle and the brackets $\langle\rangle$ indicate the average over several realizations.

In order to measure the integrated response function $\chi(t+t_w, t_w)$, we make a copy of the system at time t_w and apply to it a small random perturbation, varying the diffusion probability of each particle from $p = \frac{1}{4}$ to $p^\epsilon = \frac{1}{4} + f_i^r \cdot \epsilon$, where $f_i^r = \pm 1$ is a random variable associated to each grain independently for each possible direction ($r = x, y$), and ϵ represents the perturbation strength. For a constant field we obtain (see also [4, 5, 18]):

$$\chi(t+t_w, t_w) \;=\; \frac{1}{2\epsilon N}\sum_{i=1}^{N}\sum_{r=x,y}\langle f_i^r \cdot \Delta r_i(t+t_w)\rangle$$

where $\Delta r_i(t+t_w) = r_i^{repl}(t+t_w) - r_i(t+t_w)$ is the difference between the displacements taking place in the two systems evolving with the same succession of random numbers. In this letter we present the results obtained with a perturbation strength $\epsilon = 0.005$, having checked that for $0.002 < \epsilon < 0.01$ non-linear effects are absent.

If the system was in equilibrium we would expect B and χ to be linearly related by

$$\chi(t+t_w, t_w) = \frac{X_{dyn}}{T_d^{eq}} B(t+t_w, t_w), \tag{1}$$

where X_{dyn} is the so-called Fluctuation-Dissipation Ratio (FDR) which is unitary in equilibrium. Any deviations from this linear law signals a violation of the Fluctuation-Dissipation Theorem (FDT). Nevertheless it has been shown, first in mean-field models [20], then in various simulations [21, 22] how in several aging systems violations from (1) reduce to the occurrence of two regimes: a quasi-equilibrium regime with $X_{dyn} = 1$ (and time-translation invariance) for "short" time separations ($t \ll t_w$), and the aging regime with $X_{dyn} \leq 1$ for large time separations. This second slope is typically referred to as a dynamical temperature $T_{dyn} \geq T_d^{eq}$ such that $X_{dyn} = T_d^{eq}/T_{dyn}$ [23].

In our case, as the density increases, an aging behaviour is obtained: the system falls out of equilibrium and $\rho_{mob}(t)$ gets smaller than the corresponding value at equilibrium [5]. Accordingly, violations of (1) are expected.

If the compaction process is stopped at a certain time t_w, the system relaxes toward equilibrium and one obtains a time-translation invariant behaviour for χ and B; this is the so-called regime of interrupted aging which features an increase of ρ_{mob} to its equilibrium value and a single linear relation for the χ vs. B parametric plot. These measures therefore give us the value of the equilibrium fluctuation-dissipation ratio, T_d^{eq}, which does actually not depend on the density reached at t_w.

If, on the other hand, the compaction process is not stopped, the system features an aging behaviour and the χ vs. B parametric plots, displayed in figure 1, show two different linear behaviours: after a first quasi-equilibrium regime in which the plot has slope T_d^{eq}, a violation of FDT is observed, with the existence of a dynamical temperature T_{dyn} which depends on t_w and therefore on the density. We obtain in particular $X_{dyn}^1 = 0.646 \pm 0.002$, $X_{dyn}^2 = 0.767 \pm 0.005$, $X_{dyn}^3 = 0.784 \pm 0.005$ at $t_w^1 = 10^4$, $t_w^2 = 3 \cdot 10^4$, and $t_w^3 = 5 \cdot 10^4$.

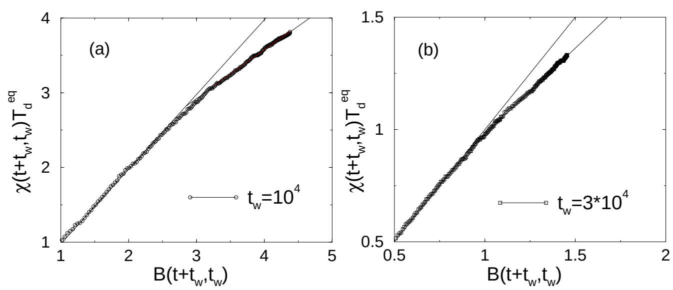

FIG. 1: Einstein relation in the Tetris model: plot of the mobility $\chi(t_w + t, t_w)T_d^{eq}$ vs. the mean-square displacement $B(t_w + t, t_w)$, for $t_w^1 = 10^4$ and $t_w^2 = 3 \cdot 10^4$. The unitary slope of the full straight line corresponds to the equilibrium case, obtained for the dynamics at constant density (interrupted aging).

We are now able to compare the values of the dynamical measures with the outcome of Edwards' measure. The construction of the equilibrium and Edwards' measures has been described in [5]. In particular, an efficient sampling of the blocked configurations, and therefore Edwards' measure, is obtained by the use of an auxiliary model whose energy is defined to be the number of mobile particles: the introduction of an auxiliary temperature and an annealing procedure then yields configurations with no mobile particles. Having computed equilibrium and Edwards' entropies as a function of density, as in [4, 5], we measure the ratio of the slopes (that we denote as Edwards' ratio)

$$X_{Edw} = \frac{ds_{Edw}(\rho)}{d\rho} \Bigg/ \frac{ds_{equil}(\rho)}{d\rho}, \qquad (2)$$

which is plotted in figure (2). This ratio approaches 1 as $\rho \to 2/3$, since at the maximum density all configurations become blocked and therefore equilibrium and Edwards' measures become equivalent.

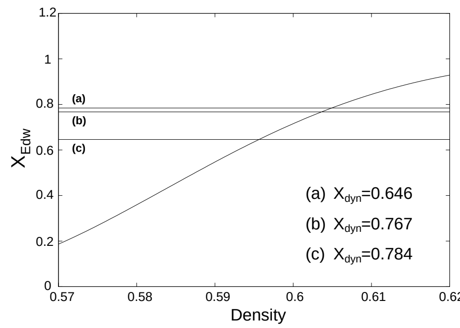

FIG. 2: Edwards' ratio X_{Edw} as a function of density. The horizontal lines correspond to the dynamical ratios X_{dyn}, measured (from bottom to top) at $t_w = 10^4$, $3 \cdot 10^4$, $5 \cdot 10^4$ and determine the values $\rho_1 \approx 0.596$, $\rho_2 \approx 0.603$, $\rho_3 \approx 0.605$, to be used in the comparison with the results reported in Fig. 3.

The values of the dynamical Fluctuation-Dissipation ratio are also reported in the same figure (with no error bars since they are too small) and yield the following densities: $\rho_1 \approx 0.596$ for $t_w^1 = 10^4$, $\rho_2 \approx 0.603$ for $t_w^2 = 3.10^4$, $\rho_3 \approx 0.605$ for $t_w^3 = 10^5$. On the other hand, the evolution of the density of the system during the measurements is reported in figure (3).

	X_{dyn}	**density**	**density interval**
$t_w = 10^4$	0.646	0.596	$[0.584, 0.597]$
$t_w = 3 \cdot 10^4$	0.767	0.603	$[0.599, 0.605]$
$t_w = 5 \cdot 10^4$	0.784	0.605	$[0.603, 0.606]$

TABLE I: Fluctuation-Dissipation Ratio (X_{dyn}) as obtained from numerical data fits with the corresponding densities obtained from figure (2). The last column reports the density intervals explored during the compaction dynamics (starting from the times where deviations from equilibrium become evident) for $t_w = 10^4$, $3 \cdot 10^4$, $5 \cdot 10^4$.

Since the measurements are performed *during* the compaction, the density is evolving, going from $\rho(t_w)$ to $\rho(t_w + t_{max})$. In each case, we obtain that indeed $\rho_i \in [\rho(t_w^i), \rho(t_w^i + t_{max})]$ where we have denoted with ρ_i the densities obtained from figure (2) for different values of t_w ($i = 1, 2, 3$). More precisely, ρ_i is very close to $\rho(t_w^i + t_{max})$. This is to be expected since the measure of the FDT violation is made for times much larger than t_w^i and, since the compaction is logarithmic, the system spends actually more time at densities close to $\rho(t_w^i + t_{max})$ than to $\rho(t_w^i)$.

The validation of Edwards' hypothesis in various model systems has made important steps forwards recently; here we have focused, for a model with only geometrical constraints, on the definition of a dynamical temperature and on its link with Edwards' measure. While the

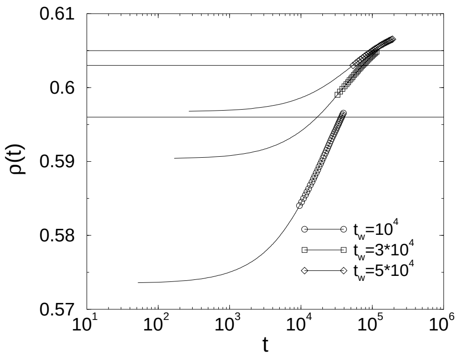

FIG. 3: Evolution of the density during the measurements of χ and B, for $t_w = 10^4,\ 3 \cdot 10^4,\ 5 \cdot 10^4$. The evolution during the quasi-equilibrium part is plotted with lines, and during the violation of FDT with symbols. The horizontal lines correspond to the densities ρ_1, ρ_2, ρ_3 from Fig 2.

density increases, the measured dynamical temperature decreases, following closely the ratio between the equilibrium and the Edwards' entropies, the latter being obtained through a flat sampling of blocked configurations. While Edwards' proposal is supposed to be only valid asymptotically, i.e. when one-time quantities are almost stationary, our study clearly shows that it actually yields good results even in a pre-asymptotic regime, when the density is still evolving a lot.

Two remarks are in order. It is interesting to investigate the limits of validity of Edwards' approach. Though in this letter we have shown that Edwards' measure works nicely in the idealized case of an homogeneously compacting system, it is important to consider the case of a compacting system under gravity, i.e. with a preferential direction. We shall report about this in [18]. Another crucial point concerns the fact that the dynamically defined effective temperature could a priori depend on the observables used for the measure of Fluctuation-Dissipation relations. Its interpretation as a temperature in a thermodynamical sense would then be questioned. While the effective temperature is known to be observable independent for mean-field models, this question has been addressed only recently in realistic models: two recent studies on sheared (stationary) thermal [12] or athermal [13] systems show the consistency of various definitions [24]. Our results complement these studies by allowing to relate the value of T_{dyn} to a static measure. Moreover, the observable-independence character of T_{dyn} in our case will be checked in [18], by considering systems consisting of 2 types of particles. In this respect, the presence of a preferential direction could imply limitations; for sheared, stationary systems, a preferential direction exists, but only measures along orthogonal directions have been performed [8, 12, 13, 25]. Acknowledgments This work has been partially supported by the European Network-Fractals under contract No. FMRXCT980183.

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